REPORT DOCUMENTATION PAGE

Form Approved
OMB NO. 0704-0188

1. AGENCY USE ONLY (Leave Blank)

2. REPORT DATE
September 2000

3. REPORT TYPE AND DATES COVERED
Final

4. TITLE AND SUBTITLE
Propagation of Waves in Optical and Photonic Media

5. FUNDING NUMBERS
DAAH04-96-1-0157

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8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES)

U. S. Army Research Office
P.O. Box 12211
Research Triangle Park, NC 27709-2211

10. SPONSORING / MONITORING AGENCY REPORT NUMBER

ARO 35664.8-MA

11. SUPPLEMENTARY NOTES

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12 a. DISTRIBUTION / AVAILABILITY STATEMENT

Approved for public release; distribution unlimited.

12 b. DISTRIBUTION CODE

13. ABSTRACT

The most direct and immediate benefit to the Army from the research under the grant of this report, is the development of a fast, efficient numerical code for transmission computations in two dimensional photonic crystals with or without defects and with or without dielectric losses. The code has been used in joint work with H. Everitt (ARO and Duke, Physics) and his group who performed physical experiments towards the manufacture of a photonic crystal laser; the resonant frequencies and corresponding quality numbers computed by our code have provided crucial help to the experimental work and were in very good agreement with the experimental values.

We have currently made the code available to Dr. Everitt and his group. It is being used by members of his lab. We are in the process of making minor changes in the code that will

14. SUBJECT TERMS

20001122 016

15. NUMBER OF PAGES

16. PRICE CODE

17. SECURITY CLASSIFICATION OR REPORT	18. SECURITY CLASSIFICATION ON THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT
UNCLASSIFIED	UNCLASSIFIED	UNCLASSIFIED	UL

NSN 7540-01-280-5500

Standard Form 298 (Rev.2-89)
Prescribed by ANSI Std. 239-18
298-102

enable us to make it available to all the scientists in the Army who wish to use it.

The work on transmission through a discrete periodic medium, raises the possibility of using photonic crystals in efficient Second Harmonic Generation. We believe that our continued research on the project will provide specific parameters that can be used in the fabrication of such a device by Army scientists.

TITLE

PROPAGATION OF WAVES IN OPTICAL AND PHOTONIC MEDIA

TYPE OF REPORT (TECHNICAL, FINAL, PROGRESS)

FINAL REPORT

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DATE

September 11, 2000

U.S. ARMY RESEARCH OFFICE
P.O. Box 12211
Research Triangle Park, NC 27709-2211

CONTRACT/GRANT NUMBER

DAAH 04-96-1-0157

INSTITUTION

DUKE UNIVERSITY

RESULTS

Linear

Our goal has been

- the use of analysis for the creation of efficient codes for the solution of Maxwell's equations in a complicated two dimensional environment involving spatially periodic dielectric structures.
- the use of these codes in the analysis of EM propagation through such structures in the presence of various types of defects.

We have obtained the following results.

Completed Projects

We have created a code for 2-D EM transmission through photonic crystal structures that are periodic in one direction and repetitive but finite in the other.

- Our computation is in the frequency domain and implements the boundary integral/boundary element method. The 2-D Maxwell equations are reduced to a set of integral equations on the 1-D interface (boundary) of the two dielectrics; we use a 1-D finite elment method to solve the integral equations. To accellerate Green's function convergence in regimes where it is slow, we use the Ewald representation of the Green's function.
- The code applies equally well to both lossless and lossy dielectrics.
- The code can calculate structures with cavity or other kind of defects that are of technological interest. We have studied in detail the variation of the resonant frequencies and corresponding quality factors versus cavity size in both lossy and lossless Fabry-Perot photonic crystal structures. We have derived a basic design rule for choosing the number of dielectric rod rows to attain a maximal quality factor, given the loss tangent of the dielectric material.

Projects in which significant progress has been made

- A drawback, generic to the boundary integral method, is that the matrix in the resulting linear system is full. We have designed a modified faster algorithm that (a) results in a banded matrix that is of a somewhat larger size than the full matrix of the original method and (b) makes the calculation of the matrix more efficient. With the new code, we are able to decrease the computation time drastically. For example, a specific computation (hexagoanal structure, eight rods, single frequency 16 elements

per rod) that took 1.5 minutes in the original approach, is done in 2.7 seconds with the fast method. We accompish this by utilizing the separability properties of the Green's function. We introduce additional auxilliary unknowns that lump influences from substructures of the crystal and by treating long range and short range influences in a different way. Our final matrix in this approach is larger because it includes the new variables, but it is much sparser. This improved code is currently under development.

- The original natural formulation of the boundary integral equations leads to a Fredholm system of the first kind. The inverse operator is unbounded and the inversion is theoretically not stable. Yet, the logarithmic singularity of the corresponding distribution kernel allows a numerically fairly stable inversion by a direct scheme. Stability should become a serious issue in this case for very large systems, that do arise in practice because the eigenvalues of the Fredholm operator converge to zero. Anticipating this difficulty, we have obtained an efficient way to write the boundary integral equations as a system of the second kind, that will allow us to investigate possible faster iterative inversion methods.

Projects in an early stage that started during the period of this grant

- We have started implementing our code in numerical experiments over various types of defects. Our goal is to identify interesting and novel types of resonances that may be useful in optical devices. An interesting resonance occurs in an array of 2-D photonic crystal blocks separated by passages along the direction of the incident EM radiation. In the bandgap of the crystal, we find resonant frequencies of enhanced transmission corresponding to "waveguide" modes of the passage. In other words, the field is concentrated in the passage areas and the interior of the crystal is dark. We also find a different more interesting kind of resonance, still in the bandgap, in which the passages are dark, and the field is concentrated in the interior of the crystal (collaboration with Mansoor Haider and Stephen Shipman). In current research, we are analyzing these results and also performing further numerical experiments.

- We have begun the development of a full 3-D boundary integral code (PhD thesis: Andrew Barnes). The mathematical analysis for this system is complete and we have begun the coding.

- in order to study dynamic phenomena, we need a code in real time. We have started work on a finite difference-time domain (FDTD) code in 2-D (will proceed with 3-D shortly; PHD thesis of Christopher Hale, also supported by AASERT).

Nonlinear: nonresonant and resonant transmission in a one dimensional discrete periodic medium.

We analyze rigorously a chain of identical nonlinear inductors connected in series at nodes that are grounded through capacitors of two types. The capacitors alternate along the chain

of inductors and this gives the medium its periodice nature. The circuit equations of the structure are identical to the equations of the nonlinear diatomic chain. We find that a small optical nonlinearity displays dramatic leading order effects in transmission through the medium through the mediation of resonances.

Project Completed: nonresonant transmission

We have constructed the nonlinear analogue of plane waves along the medium at nonresonant frequencies. To do this we

- We seek a solution of two nonlinearly interacting traveling periodic waves, one on the odd indexed and the other on the even indexed nodes.
- We reduce the nonlinear system to an infinite set of equations for the Fourier coefficients of these waves.
- We apply bifurcation theory, in particular the Lyapounov Schmidt decomposition, in which the system is decomposed to a finite dimensional problem in the null space of the linearized operator and an infinite problem in the orthogonal complement. The solution of the latter, controlled by the use of the infinite dimensional implicit function theorem, and inserted in the finite system, provides the bifurcation equation. This is the **nonlineardispersionrelation** that relates the frequency with the wavenumber and with the amplitude of the fundamental. The total energy of the harmonics is asymptotically of higher order than this of the fundamental. The amplitude of the fundamental is the asymptotic paramenter.

Project Completed: Second harmonic generation (SHG) through 1:2 resonance

In the analysis of the nonresonant case, the null space of the linearized operator is one dimensional. In an analysis that is uniform near the 1:2 resonance, the null space is two dimensional. The fundamental (first harmonic) and the second harmonic arise with amplitudes of the same order. The bifurcation system gives two relations each involving the frequeny, the wavenumber and the amplitudes of the first and second harmonics. Using the wavenumber and the amplitude of the **second** harmonic as our basic variables, we show that in solution space, there is a continuous connection between a solution of almost entirely fundamental frequency to a solution that has essentially all its energy in the second harmonic and zero energy in the firs harmonic.

The natural followers of these projects namely

- numerical experiments to probe dynamic SHG at the 1:2 resonance
- the analysis of the full multilayer photonic crystal for SHG.

are being pursued in the current grant of the PI. The latter project investigates the photonic crystal as an efficient frequency doubling device.

Project completed: Rigorous calculation of scattering data for the nonlinear Schrödinger equation (NLS)

The NLS equation describes solitonic transmission in fiberoptic communication and is genertally encountered in propagation through nonlinear media. It will play a serious role in wave propagation through a photonic crystal. One of its most important aspects is the modulational instability that it displays. Regular wavetrains are unstable to modulation and break up to more complicated structures.

The NLS equation is solvable in theory by the method of inverse scattering, which utilizes spectral information of a linear operator, the Lax operator, associated with the unknown solution. In the first step of the method, the initial spectral data of the Lax operator are calculated from the solution which is known at time zero. The spectral data evolve in a trivially simple way, and the remaining step is to recover the unknown solution at time t from the spectral data at time t, a process known as inverse scattering. In the case of NLS, the required spectral data corresponding to an initial condition that should naturally lead to modulated waves, is hard to calculate. Furthermore, given the instability of the problem it is not clear to what extent the solution is drastically affected by approximations in the calculation.

We have developed (collaboration with A. Tovbis) an example in which the derivation of the spectral data is explicit. We employ the use of hypergeometric function theory to establish the connection formula needed to relate the asymptotic data of the eigenfunctions for asymptotically large positive and large negative values of the space variable. Our calculation has yielded the interesting fact that the spectrum may or may not have a discrete part according to the value of a certain parameter in the initial data.

In continuation of this work we are currently working on the inverse scattering step for the calculation of the solution.

TECHNOLOGY TRANSFER

The most direct and immediate benefit to the Army from the research under the grant of this report, is the development of a fast, efficient numerical code for transmission computations in two dimensional photonic crystals with or without defects and with or without dielectric losses. The code has been used in joint work with H. Everitt (ARO and Duke, Physics) and his group who performed physical experiments towards the manufacture of a photonic crystal laser; the resonant frequencies and corresponding quality numbers computed by our code have provided crucial help to the experimental work and were in very good agreement with the experimental values.

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PUBLICATIONS

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- S. Venakides, M. Haider, V. Papanicolaou *Wave Propagation in Photonic Crystal Models*, Proceedings of International Conference in Perdika, Greece, to appear.

PARTICIPATING PERSONNEL

The personnel listed (a) belonged to the Duke Math Department faculty or graduate student body for some period during the grant, and (b) participated in the research projects of the grant. An asterisk (*) by a researcher's name indicates that this person did not receive any pay from the grant.

- Stephanos Venakides, PI

- Stephen Shipman, Assistant research professor, Duke Univ. Dept of Math.

- Mansoor Haider*, Postdoc, Duke U., currently Asst. Prof. NCSU, Dept. of Math.

- Anne-Marie Filip, Graduate student in mathematics, PhD May 1997, currently Asst. Prof. Ryerson U., Toronto, Canada.

- Anna Georgieva, Graduate student in mathematics, PhD December 1997, currently Visiting Prof. NJIT, Dept. of Math.

- Andrew Barnes*, Graduate student in mathematics
- Christopher Hale, Graduate student in mathematics (funded by AASERT)

BIBLIOGRAPHY

see list of publications